



Curtin University

WA School of Mines: Minerals, Energy and Chemical Engineering

1st Annual WASM: MECE HDR Conference: Transforming the Future

Friday 22 July 2022 | Curtin University (Perth Campus)

Conference Proceeding

Conference Chair: A/Prof. Hussein Znad

Conference Co-Chair: Prof. Michael Hitch

Edited By

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Acknowledgement to Country (Boodja)

Curtin University would like to pay our respect to the Aboriginal and Torres Strait Islander members of our community by acknowledging the traditional owners of the land on which the Bentley Campus is located, the Wadjuk people of the Nyungar Nation; and on our Kalgoorlie Campus, the Wongutha people of the North-Eastern Goldfields.

Special thanks to the Organising committee

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Conference Program

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08:30-09:00	Registrations
Opening Session	
09:00-09:05	Conference open and welcome to Country A/Prof. Hussein Znad, Conference chair & School DGR
09:05-09:15	Opening address Prof. Michael Hitch, WASM:MECE Head of School & conference co-chair
09:15-09:25	Opening address Prof. Kate Trinajstic, Dean of Research- Faculty Science & Engineering
Keynote Presentations	
09:25-09:50	Carbon to Products: Aiming to recycle greenhouse gases into useful products Amanda Panting, Carbon Capture and Utilisation Manager in Woodside Energy Group.
09:50-10:15	Looking forward – Mining Green Mr. Tony Tang- General Manager Technology and Process Development, Blackstone Minerals
10:15-10:40	A PhD Journey: From Traditional to Future Industries Dr. Sofia Hazarabedian, Energy Transition Advisory, KBR
10:40-11:05	MPS's pathway of commercialising the GlyLeach/GlyCat technology from lab to industry licences Mr. Ivor Bryan, Managing Director, Mining & Process Solution (MPS).
11:05-11:30	Technology Augmentation and The Energy Transition Mr. Andrew Tran, Production and Processing Engineering Team Lead at Schlumberger Australia
GROUP PHOTO	
11:30-11:45	Coffee Break
Oral Presentations - Session A	
Session Chairs: A/Prof Hari Vuthaluru & Dr. Chunyan Fan	
11:45-12:00	Gravity Recovery of Gold: A Review <u>Jessica Frigger</u> , E. Avelar, T.D.H. McGrath, C. Aldrich, A.R. Bax and W.P. Staunton
12:00-12:15	Effect of Reboiler Operation on thermally degraded MEG Thermodynamic Inhibition <u>Dana Badi</u> , Ammar Al Helal, Barasha Deka, Chris Lagat, Chi Phan, Ahmed Barifcani
12:15-12:30	Understanding Stress Corrosion Cracking of Corrosion Resistant Alloys Using Data Science <u>Abraham Rojas Zuniga</u> , Sam Bakhtiari, Victor Calo, and Mariano Iannuzzi
12:30 -1:30	Lunch Break

Oral Presentations - Session B	
Session Chairs: Dr. Tejas Bhatelia	
1:30-1:45	B-prompted Ni-Co catalysts for dry reforming of methane reaction <u>MD Shakir</u> , Siddhartha Sengupta, Apurba Sinhamahapatra, Shaomin Liu, Hari Vuthaluru.
1:45-2:00	Prospects for improved reaction kinetics for low CO₂ emissions and high syn gas production during Australian low-rank coal gasification <u>Manoj Kumar Jena</u> , Vineet Kumar and Hari Vuthaluru
2:00-2:15	Data Analytics integration with multiscale characterisation of shale: A workflow for successful hydrocarbon exploration from gas shale reservoirs <u>Muhammad Atif Iqbal</u> , Reza Rezaee, Gregory Smith
2:15 -2:30	Coffee Break
Oral Presentations - Session C	
Session Chairs: Dr. Arash Arami-Niya	
2:30-2:45	Natural Hydrogen Prominence and Controls of Distribution in the Earth Crust <u>Vitaly Vidavskiy</u>
2:45 - 3:00	Benzoxazine resin as a sandstone surface wettability modifier <u>Gonzalo Mauricio Ceron Lopez</u> , Matthew B. Myers, Quan Xie, Colin D. Wood, Ali Saeedi
3:00 - 3:15	Computational modelling of reactive processes in lithium-metal batteries <u>Marcos Exequiel Arguello</u> , Nicolas Agustin Labanda, Monica Gumulya, Jos Derksen, Ranjeet Utikar, Victor Manuel Calo
3:15 - 3:30	Optimised Process for Methanol Production via Bi-reforming Syngas <u>Christopher Acquarola</u> , Milinkumar Shah, Tejas Bhatelia, Vishnu Pareek and Min Ao
3:30 - 3:45	Viscoelastic creep/stress relaxation to predict S_{hmin} magnitude in deep sedimentary rocks <u>Partha Pratim Mandal</u> , Reza Rezaee and Joel Sarout
3:45 - 4:00	Coffee Break
Oral Presentations - Session D	
Session Chairs: Dr. Yun Yu	
4:00 - 4:15	<i>Dual-phase with Ni addition: microstructure design and hydrogen embrittlement resistance evaluation</i> <u>Esteban Rodoni</u> , Tom Depover, Mariano Iannuzzi
4:15 - 4:30	EXPERIMENTAL HYDRAULIC FRACTURING TECHNIQUE FOR HARD ROCK IN-SITU RECOVERY ENHANCEMENT <u>Hongyi Sun</u> , Mohammad Sarmadivaleh
4:30 - 4:45	Long-and Short-term Strategies for Estimation of Hydraulic Fracturing Cost Using Fuzzy Logic <u>Hyunjun Im</u> , Hyongdoo Jang, Erkan topal, and Micah Nehring
4:45 -5:45	Coffee Break & Poster Presentations - Session E

Poster Presentations - Session E	
P-1	Water Shutoff in High Permeability Sandstone Gas Reservoirs: Role of Additives and Fluid Flow Rate <u>Faaz Al-shajalee</u> , Colin Wood, and Ali Saeedi
P-2	An investigation of <i>in situ</i> formation of metal pyrophosphates (MP₂O₇, where M = Sn, Ti and Zr) in PA/PBI based composite membrane in high-temperature polymer electrolyte membrane fuel cells <u>Zehua Wang</u> , Zongping Shao and San Ping Jiang
P-3	Maleic anhydride based polymeric additives for the control of flow assurance problem of gas hydrate formation <u>Barasha Deka</u> , Rohit Sharma, Vikas Mahto, Ahmed Barifcani, Hari Vuthaluru
P-4	CFD Analysis of Frost Growth under Various Conditions using Mass Transfer Theory <u>Joshua C. Q. Wong</u> , Vishnu K. Pareek, Biao Sun
P-5	Effect of Wire Shape and Size in Droplet Capture <u>Muhammad Dary Mahadika Priyambodo</u> , Tejas Bhatelia, Milinkumar Shah, Biao Sun, and Vishnu Pareek
P-6	Natural Hydrogen Prominence and Controls of Distribution in the Earth Crust <u>Vitaly Vidavskiy</u>
P-7	Comparison study of methanol production via CO₂ hydrogenation and syngas <u>Kemal F Hastadi</u> , Tejas Bhatelia, Biao sun, Jim Patel
P-8	Adsorption of CO₂/CH₄ Mixtures in Activated Carbon <u>Allan Hua Heng Sim</u> and Chunyan Fan
5:45 - 6:00	Closing session & Awards giving
6:00 -7:30	Drinks, Nibbles and Networking

Conference Abstracts

Keynote presentations

Carbon to Products: Aiming to recycle greenhouse gases into useful products

Amanda Panting, Carbon Capture and Utilisation Manager in Woodside Energy Group.

Abstract

Woodside is looking to avoid emissions by design out, reduce emissions by operating out and offset/abate the emissions it can't eliminate. Carbon to Products (C2P) which recycles greenhouse gases (CO₂ and CH₄) and transforms them into value-added products, is part of the Woodside Carbon Management Plan. C2P is an emerging field and the technologies are at various stages of maturity. Woodside C2P team screens and evaluates various technologies, piloting the more mature technologies and partnering with technology providers and universities to develop promising technologies that are less mature. PhD graduates in the team play key roles in these activities.

Biography: Amanda Panting is currently the Carbon Capture and Utilisation Manager in Woodside Energy Group, New Energy Business. She leads a team of 11 people looking at how to convert greenhouse gases (i.e. CO₂ and methane) into value-added products. She has a Geophysics background, with over 20 years' experience in exploration, development and business. For the last five years she has been leading Technology teams in Geoscience, Technology and New Energy.

Looking forward – Mining Green

Mr. Tony Tang- General Manager Technology and Process Development, Blackstone Minerals

Biography: Mr Tang graduated from Curtin University, a chartered professional member of FAusIMM (CP), and has been working in the resources sector over 25 years.

Mr Tang's experience spans laboratories, operations, engineering consultancies – projects development, studies, EPC, EPCM, sustaining capitals and commissioning.

Since 1995, Mr Tang extensively involved in multiple second generation HPAL nickel and cobalt laterite projects. Mr Tang worked at Murrin Murrin Operations for nearly a decade where he involved in commissioning, operations, plant optimisation and ongoing R&Ds projects.

Since 2007, Mr Tang worked with top tier engineering consultancy firms where he extended his engineering excellence in studies, detailed design and projects execution. Mr Tang led many complex chemical processing projects in Rare Earth, Lithium, Gold, Nickel, Cobalt, Scandium, and minerals sand.

A PhD Journey: From Traditional to Future Industries

Sofia Hazarabedian, Energy Transition Advisory, KBR, Perth, WA, Australia, sofia.hazarabedian@kbr.com

Abstract: Opportunities to produce a positive impact and foster a cleaner and fairer world are escalating rapidly. The beauty of the doctorate is that it shapes graduates with valuable skills to solve the biggest challenges of the new era. Each PhD journey is unique, diversifying the graduates' profiles and enriching the workforce. In this presentation, Sofia Hazarabedian will share her PhD experience and how it helped her migrate to future industries development at KBR. Particularly, she will present an overview of her PhD on traditional sectors and KBR's role in a critical mineral production site as a case study. Lastly, she will share her view on the central role of Materials Science and Engineering in enabling the transition to sustainable economic growth.

Biography: Sofia Hazarabedian is an Energy Transition Consultant at KBR, a technology developer providing sustainable solutions around the world. She is a Materials Engineer from the Sabato Institute, Argentina, and a recent PhD graduate from the Curtin WA School of Mines. Her doctorate focused on the physical metallurgy of materials susceptible to hydrogen embrittlement used to produce resources.

MPS's pathway of commercialising the GlyLeach/GlyCat technology from lab to industry licences

Mr. Ivor Bryan, Managing Director, Mining & Process Solution(MPS).

Biography: Ivor has over 35 years' experience in the mining industry with executive management roles in operations, project management, and consulting. During his career, Ivor has managed the development of a large underground mining operation at Olympic Dam, led multi-disciplinary teams on resource development projects in both Australia and overseas, and been involved in numerous feasibility studies for Australian and international clients. He has a first class honours degree in Mining Engineering obtained from the University of Sydney, a first class mine managers certificate of competency and has completed executive development courses with the business school at the University of Western Australia.

Technology Augmentation and the Energy Transition

Andrew Tran, Production and Processing Engineering Team Lead at Schlumberger Australia

Abstract: With the transition to new energy sources comes an additional demand on energy storage solutions that can meet instantaneous demand for energy in the way that coal, oil and gas can. One of the leading technologies expected to be a crucial component of this energy transition is the production, transportation and storage of hydrogen. This talk will explore some of the technologies and approaches we are currently using in exploring the energy transition.

Biography: Andrew Tran graduated from Curtin University with a bachelor degree in Chemical Engineering and master degree in Petroleum Engineering from the University of Western Australia. He has been working as a Production Engineer with Schlumberger Australia since 2010. During his time in Schlumberger he has performed projects on well test analysis, production accounting, well workover recognition, and production system optimisation and integrated asset modelling. Before he joined Schlumberger, he was an Asset Engineer with an operating company where he was executing compliance and maintenance projects on hydrocarbon assets based in Western Australia's North West.

Oral presentations

Gravity Recovery of Gold: A Review

J. Frigger¹, E. Avelar², T.D.H. McGrath³, C. Aldrich⁴, A.R. Bax⁵ and W.P. Staunton⁶

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Presenter: Jessica Frigger

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Abstract: Batch centrifugal concentrators such as Knelson's are commonly used to recover gold from free-milling gold ores because they are highly efficient and are a low-cost method for producing a net recovery benefit for the plant. Free milling gold ores achieve a recovery of over 90% with standard cyanidation. However, few new free-milling gold ore bodies high and coarse gravity recoverable gold content are being discovered. Many gold plants now treat ores that are somewhat complex in nature, characterised by high-density gangue and/or competing components, such as silver and copper. Gravity recovery of gold from complex ores does not have a clear method for detailed characterisation and recovery can be less than what would be expected. Many operators rely on manufacturers' recommendations or best practice to operate their gravity circuits. Characterising complex gold ores for their amenability to gravity recovery methods, as well as optimising plant and machine parameters for operating the gravity circuits could improve net gold recovery and decrease operating costs. This presentation reviews the available literature for gravity recovery of gold from complex ores with high-density gangue. A summary of current operational practice for selected gold plants operating gravity circuits with complex ore-based feed is also presented.

Effect of Reboiler Operation on thermally degraded MEG Thermodynamic Inhibition Performance

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Presenter: Dana Badi

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Abstract: Mono ethylene glycol (MEG) has been used as a common thermodynamic hydrate inhibitor to control gas hydrate issues in the offshore industry. Owing to its high quantities usage and environmental effect, MEG is usually regenerated and recycled in a reboiler distillation system to be injected back. Surplus water is removed from MEG by exposing MEG to higher temperatures to increase MEG purity, and as such MEG thermal degradation occurs due to the generation and accumulation of organic acids including glycolic, acetic and formic acids in the reboiler lean MEG products. The accumulation of these organic acids will decrease the MEG thermodynamic inhibition performance and more recompensed fresh MEG amounts are needed for top up. The objective emphasizes on determining the extent of the MEG degradation products accumulation and optimizing the thermodynamic hydrate inhibition performance of these thermally degraded MEG products.

The results indicate that the longer reboiler operation of 6.0 hrs at higher MEG concentration of 80.8 vol % has resulted into raising the hydrate dissociation temperature by an average of 1.4 °C compared to 0.9 °C compared to lower MEG concentration of 40.2 vol % at the same retention time. This is due to higher organic acids accumulation which lowers the MEG inhibition performance. The allowable amounts of the organic acids accumulation in the lean MEG product are proposed to ensure the MEG degradation levels are reduced to optimize the efficiency of MEG as a thermodynamic inhibitor.

Understanding Stress Corrosion Cracking of Corrosion Resistant Alloys Using Data Science

Abraham Rojas Zuniga¹, Sam Bakhtiari², Victor Calo³, and Mariano Iannuzzi⁴

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Presenter: Abraham Rojas Zuniga

Corrosion Engineering/ Western Australian School of Mines and Curtin Corrosion Centre/ Curtin University, Bentley, Western Australia, Australia, abraham.rojaszuniga@postgrad.curtin.edu.au.

Abstract: Corrosion-resistant alloys (CRAs), such as stainless steel and nickel-based alloys, are essential for operating in severe industrial environments. Due to their high mechanical properties and low corrosion rates, some CRAs can provide long lifetimes to relevant metallic components in a broad range of environments, many encompassing elevated temperatures and stresses, corrosive species, or both. Nonetheless, CRAs are susceptible to environmentally assisted degradation; principally, stress corrosion cracking (SCC).

Fundamentally, the synergistic interactions of mechanical stresses and corrosion-oxidation reactions induce SCC; the main failure cause of metallic materials. SCC is often difficult to detect, and in turn poses significant challenges to material selection and reliability engineering across various industry sectors, such as chemical processing, oil and gas, and power generation. While considerable research has been devoted to examining SCC, a thorough understanding of its underlying mechanisms is still elusive. Therefore, there is a need for a framework and predictive tools to reliably assess the associated SCC risks.

SCC is a highly complex process involving coupled electrochemical and solid-state reactions, where several interplaying factors may directly influence the SCC behaviour. In this work, we use data-centric approaches to predict SCC risks and severity; in particular, we implement machine learning (ML) techniques, as well as probabilistic graphical methods (PGM), namely Bayesian networks (BNs). These data-driven approaches have been found optimal to analyse the high number of variables involved in SCC, such as metallurgical features and environmental conditions, and stress levels.

This presentation summarises the application of BNs and ML methods for interrogating the influence of metallurgical factors (i.e., composition, heat treatment, strength, and fracture toughness) on the SCC susceptibility in chloride-rich systems. Here, we explore in detail the data from the widely known “Copson curve” to quantitatively determine the effects of nickel on the resistance to SCC.

Notably, we demonstrate the advantages of employing feature extraction algorithms, i.e., t-distributed stochastic neighbour embedding (t-SNE) to identify patterns in data, and effectively examine the failure trends. In addition, this study will present a new regression model based on extreme gradient boosting (XGBoost), which evaluates the SCC susceptibility as a function of fracture toughness, the chemical composition of alloys, and stresses levels. By way of validation, the results obtained from the XGBoost model are also compared through probabilistic studies using BNs.

In this work, we suggest a new interpretation of fracture toughness as a key parameter to quantify the SCC susceptibility of CRAs exposed to high chloride concentrations. More importantly, we provide a more detailed analysis of the effect of nickel to reduce SCC susceptibility, which remains unclear since its first observation was reported by Harry Copson in 1959.

B-prompted Ni-Co catalysts for dry reforming of methane reaction

MD Shakir^{1,2}, Siddhartha Sengupta², Apurba Sinhamahapatra², Shaomin Liu¹, Hari Vuthaluru¹.

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Presenter: MD Shakir

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Abstract: The boron-modified catalyst synthesis method is used to prevent some long-standing problems of dry reforming of methane such as the early deactivation of the catalyst, low conversion at a lower temperature (600°C) and carbon deposition on the surface of the catalyst. This work includes a novel approach for the synthesis of boron-containing nickel-cobalt catalysts for the reforming of methane with carbon dioxide. The catalyst was synthesized by a chemical reduction method with the aid of sodium borohydride (NaBH₄). A series of different concentration of boron (0%, 1%, 2%, 3%, 5% and 7%) of Ni-based magnesium aluminate (MgAl₂O₄) supported catalyst were prepared to extract the better performance catalyst. The dry reforming of methane were performed and it appears 3% B containing Ni-B/MgAl₂O₄ catalyst were high CH₄ and CO₂ conversion where as 0% and 7% B containing catalyst were least performing catalyst. This study also verify the DFT work by Xu and Sayes that the of boron loading impact positive in terms of deactivation of catalyst. Co as second metal added over the Ni-B (3%)/ MgAl₂O₄ catalyst. A series of monometallic and bimetallic (100Ni-B, 75Ni-25Co-B, 50Ni-50Co-B, 25Ni-75Co-B and 100Co-B) catalyst were prepared with the same NaBH₄ reduction method. The catalyst were characterized by several analytical technique such as X-Ray Diffraction (XRD) patterns, H₂-Temperature programmed reduction (H₂-TPR), ICP-OES, H₂-Temperature programmed desorption (H₂-TPD) and XPS. The dry reforming of methane was conducted over MgAl₂O₄-supported Ni-B, Co-B and Ni-Co-B catalysts at 600°C in a packed tubular reactor. It was observed 75Ni-25Co-B catalyst performed well among all as TOF_{DRM} 0.300 to 0.315 after the reaction period. The spent catalyst was taken for finding out the amount of carbon deposition on the surface by elementary Analyzer and Raman spectroscopy.

Equation Oriented Modelling and the Optimization of Mixed Refrigerant Process

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Presenter: Pavas Pandey

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Abstract: New LNG facilities must meet a wider variety of process standards than they have in the past. Global increase in LNG consumption, as well as the development of feed gas sources in new and current geographic regions, are driving these requirements. In response, facilities must be built to suit a variety of new requirements. The propane pre-cooled mixed refrigerant (C3MR) technique has been the dominating liquefaction cycle for many years. Because of its adaptability, this cycle is well-suited to this ever-changing business. Using a mixed refrigerant for liquefaction & sub-cooling in a single exchanger allows the refrigerant to boil throughout a temperature range, resulting in greater efficiency where it matters most. The C3MR cycle does this by reducing the number of equipment components and control loops, all the while maintaining the highest level of efficiency. These benefits result in a plant with a low level of complexity, ease of operation, and high availability.

This research focuses on optimizing the C3MR (Propane pre-cooled mixed refrigerant) liquefaction cycle, which is frequently utilized to produce LNG on a large scale. The optimization was carried out using an Equation Oriented Modeling technique, which included a ratings-based strategy for the process's realistic design limits, such as the main cryogenic heat exchanger (MCHE) and compressors. The flow rate of mixed refrigerant, the discharge pressure of the low-pressure compressor, and the temperature distribution within the MCHE were some of the process parameters that were optimized. In contrast to a base case scenario, the suggested optimized process reduced power usage by 73.1 MJ/tonne-LNG, resulting in a 952 tonne/h decrease in CO₂ emissions and a 1.3 percent gain in exergy efficiency. This research demonstrates a feasible approach for process optimization that produces realistic and thermodynamically consistent findings, enabling for process implementation.

Biochar Based Integrated Tar Reforming for Syngas Cleaning: Insights into Volatile-Char Interactions

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Abstract: Biomass gasification is a potential and sustainable alternative employed for syngas production that can be further used for the generation of fuels or chemicals. A major roadblock in the commercialization of this process is the unavoidable generation of tar along with syngas, leading to the blockage of downstream equipment. Steam catalytic tar reforming (SCTR) using biochar emerges as the most promising thermochemical method to obtain clean gaseous products among the tested methods. Tar reforming processes conducted at typically high temperatures for syngas cleaning, fail to remove the thermally stable smaller aromatic compounds (such as naphthalene, indene, and anthracene) thereby retaining the risk of clogging downstream equipment. In this context, integration of an additional step of adsorption at a relatively lower temperature, targeting the removal of lighter tar compounds is proposed. An integrated approach for the removal of tar generated from mallee wood bio-oil, involving reforming at 750°C and adsorption at 220°C was systematically evaluated against the conventional reforming process. Herein, the current study unravels the biochar-volatile interaction of catalyst (mallee wood biochar) and tar (generated from bio-oil) during catalytic tar reforming in the presence of 15% steam. The comparative assessment included tar analysis estimating tar yield and examining tar constituents through UV-fluorescence spectroscopy, biochar structural analysis based on Raman spectroscopy supported by reactivity studies through TGA, and biochar morphological analysis by FESEM imaging and BET analysis. Tar analysis reveals a drastic drop in the two-step process by ~80%: with ~40% tar reduction in reforming and ~60 % of residual tar in adsorption. The removal of lower aromatics was confirmed through UV-fluorescence of residual tars. The Raman spectroscopy shows a growing predominance of higher aromatics in adsorbent during biochar-volatile interactions, due to adsorption of both heavy and light tar compounds. The effects of aromaticity are reaffirmed in reactivity studies by TGA. The BET results show a manifold decrease in porosity, implying coverage of the pore surface by the adsorbing species, which is also evident in FESEM images.

Prospects for improved reaction kinetics for low CO₂ emissions and high syn gas production during Australian low-rank coal gasification

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Abstract: The continuous rise in the earth's population with energy demand forces researchers across the globe to find alternative energy sources apart from fossil fuels. Although renewable sources such as biomass and bio-residue are attractive to the current world, equal attention is required to fossil fuels as it is the abundantly available resource in the earth's crust. The objective of the current study is to focus on understating the reaction mechanisms during gasification of Australian low-rank coals, i.e., Loy Yang brown coal and Collie sub-bituminous coal. Insights into mechanisms of kinetic compensation effects (KCE), which are usually observed in gas-solid heterogeneous char gasification reactions in different environments, will be discussed. An investigation of the experiment results in a pilot plant scale will also be presented. The results presented will demonstrate the impact on the production of CO/CO₂ (molar flux ratio) and the production of H₂ during char gasification (Loy Yang brown coal and/or Collie coal char) in steam and oxygen environments with the changes in particle size and reaction-controlled regime. Experimental observations revealed that the formation and consumption of active sites resulting from KCE would pave the way for the in-depth understanding of char gasification mechanisms and product gas formation. The results obtained from this study will have a significant contribution to low-rank coal from an aspect of optimizing the particle size and controlled regime under a specific gasifying environment and hence the improved yields with lower CO₂ emissions. Additionally, the findings from this study provide a knowledge base for industrial application for selecting a suitable gasifying environment along with optimal particle size in order to achieve desired product gas with reduced emissions.

Data Analytics integration with multiscale characterisation of shale: A workflow for successful hydrocarbon exploration from gas shale reservoirs

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Abstract: The heterogeneity understanding of gas shale reservoirs is very crucial and challenging for exploration and development of such big plays. A multiscale and systematic workflow is designed to characterise gas shale reservoirs by evaluating the rock types through sedimentary, mineralogical, petrophysical and statistical approaches. Different rock types are identified and classified based on core logging and laboratory based high resolution techniques. The defined rock types are integrated with petrophysical analyses, and the power of machine learning helped to identify the clusters and provided the heterogeneity understanding from log to field scale. New modified equations are derived for total porosity and water saturation estimations for gas shale reservoirs. A novel approach of defining the mechanical stratigraphy based on integration of facies, petrophysical and geomechanical properties provided new insights to propose a development plan for the gas shale reservoirs. Petrel software based 3-D modelling of facies, petrophysical and geomechanical properties (total organic carbon, porosity, water saturation, adsorbed gas, Young's modulus, Poisson's ration and brittleness index) helped to recognise the gas shale potential of Goldwyer-III shale in Canning Basin, Western Australia.

Benzoxazine resin as a sandstone surface wettability modifier

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Abstract: The use of fossil fuels for energy generation has been a major contributor to the global warming phenomenon. The emerging renewable energies combined with CO₂ removal strategies (e.g. carbon capture, utilisation and storage) are considered as the most viable options to combat global warming and its negative effects over the long term. In the meantime, replacing coal with less polluting alternatives such as natural gas could help reduce CO₂ emissions in the short term. However, for this strategy to be technically and economically viable, production from existing natural gas reservoirs needs to be boosted or at least maintained for the next several decades.

Phase trapping is a common problem that most low permeability sandstone gas reservoirs face during drilling, hydraulic fracturing, and completion operations when a volume of water invades the reservoir formation. This phenomenon negatively impacts the productivity of a gas well by drastically restricting the gas flow in the near-wellbore region. The initial water-wet condition of sandstone reservoirs is the primary reason behind such an effect. Wettability is an intrinsic property of rock that governs multiphase flow in porous media. Properties such as capillary pressure, residual saturations and relative permeability greatly depend on wettability.

This research develops a novel benzoxazine resin to alter rock wettability. The thermoresistant and environment-friendly benzoxazine monomer have been synthesised to alter rock wettability from strongly water-wet to intermediate gas-wet. The water contact angle was measured in an air-brine-rock system, obtaining intermediate wettability values of around 90°. Moreover, when treated sandstone samples were immersed in water, the rate of spontaneously imbibed water drastically decreased up to 65% compared with untreated samples. Finally, a drainage displacement process was performed at more realistic reservoir conditions of 10 MPa and 60 °C, obtaining a reduction of 10 % in the irreducible water saturation and an increment in gas relative permeability of 22 %. The results verify the efficacy of the benzoxazine chemical in altering rock wettability from strongly water-wet to less water-wet under reservoir conditions, and confirm the effectiveness of this new polymer that could be applicable for phase trapping problems in the petroleum reservoir analysis.

Computational modelling of reactive processes in lithium-metal batteries

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Abstract: Our society's continually increasing energy needs have triggered the development of improved energy storage systems. Novel materials and designs are under active research to achieve ultra-high energy density solutions. Among these, lithium metal is the most prominent negative electrode material due to its combined high theoretical energy density (3860 mAh/g) and low reduction potential (-3.04 V vs. standard hydrogen electrode). Despite these advantages, the undesired dendrites formed on the anode surface during charge cycling reduce the capacity, stability, and safety of metal anode batteries. The critical shortcoming of dendrite formation during electrodeposition processes has triggered efforts on controlling the dendritic patterns.

The investigation of lithium dendrite formation in rechargeable metal batteries becomes very challenging when based on experimental methods alone. During the past decades, various computational models have been developed to seek to understand better the fundamental mechanism of dendrite formation in metal anode batteries and guide the experiments

Here we present a computational phase-field model to describe the electrodeposition process that forms dendrites within metal-anode batteries. We derive the free energy functional model, arriving at a system of partial differential equations that describe the evolution of the phase-field, the lithium-ion concentration, and electric potential. We formulate, discretize, and solve the set of partial differential equations describing the coupled electrochemical interactions during a battery charge cycle using an open-source finite element library. The open-source library allows us to use parallel solvers and time-marching adaptivity. The conventional free energy approach is compared against the grand canonical formulation. The validity of the planar interface model is demonstrated through agreement between one-dimensional phase-field simulations and the theoretical sharp-interface Faradic reaction kinetics. Sensitivity analysis of changes in the phase-field interface thickness and under different applied voltages, as well as spatial convergence analysis of mesh-induced errors, set the groundwork for two- and three-dimensional simulations of dendritic metal electrodeposition in batteries.

We describe two- and three-dimensional simulations; these simulations agree with experimentally-observed dendrite growth rates and morphologies reported in the literature. We simulate three-dimensional spike-like lithium structures that grow under high current density (fast battery charge); these structure's growth is dangerous for battery operation. We perform single and multiple nuclei numerical experiments to study the three-dimensional distribution of the electric field and the lithium-ion concentration to understand the mechanism behind tip-growing lithium morphologies better. The analysis reveals that dendrite formation is connected to the competition between the lithium cation diffusion and electric migration forces, generating an uneven distribution of lithium ions on the electrode surface. This fact gives insight into strategies of dendrite suppression. This work constitutes a relevant step towards physical-based, quantitative models to rationalize hazardous three-dimensional dendritic patterns needed to achieve the commercial realization of lithium metal batteries.

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Optimised Process for Methanol Production via Bi-reforming Syngas

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Abstract: An optimised methanol production process via bi-reforming for industrial scale capacity 1MTPA, has been developed and presented. Furthermore, the process exhibits the second lowest resultant carbon emissions in open-source literature. Integral factors governing successful optimisation and motivation behind decreasing carbon emissions include feed ratio, temperature and pressure conditions, purge ratio and an integrated heat exchanger network. Feed ratio optimisation was carried out by investigating overall plant wide carbon emissions whilst varying methane within bi-reforming reactor. Additionally, the relative rates and extent of dry reforming, steam methane reforming and water gas shift reactions present within the bi-reforming reaction were scrutinised with varying methane ratio. A feed ratio of 3:1:2 (CH₄:CO₂:H₂O) is commonly utilised however, it was determined with a 1:1:2 ratio, overall carbon emissions can be significantly reduced due the 100% conversion of CH₄ and 44% conversion of CO₂ resulting with a H₂/CO ratio of 1.78. Unreacted CO₂ was treated by an acid gas removal unit with methyl diethanolamine and piperazine and recycled upstream before being sent to the bi-reforming reactor. Bi-reforming and methanol reactors operating conditions were determined optimal at 910 °C and 7 bar and 250 °C and 80 bar respectively. Generally bi-reforming reactors are modelled using Gibbs free energy reactors or two stage reforming reactors however a single stage plug flow reforming reactor, with catalyst and integrated kinetics have been utilised to present industrial applicability. Moreover, reaction kinetics followed Langmuir–Hinshelwood–Hougen–Watson (LHHW) kinetics. Various purge ratio percentages were investigated with 5% selected as the most suitable. The combustion of purge stream was utilised in an integrated heat exchanger network developed using aspen energy analyzer and the pinch technique. Pinch temperature was maintained at 10 °C with cold and hot pinch temperatures located at 160 °C and 170 °C. The use of 27 heat exchangers for heat recovery resulted in 221 MW of heat recovered. Resultant carbon emissions for 1MTPA methanol plant were ~0.31 tonnes CO₂/tonne of methanol, which is one of the lowest present within literature and significantly lower than comparative studies. Current work has focused on further decreasing carbon emissions with the use of thermal energy storage for low grade energy requirements including, reboiler energy and electricity duties and an electrified reformer design. Moreover, single stage bi-reforming catalyst testing has begun where experimental results will be compared to simulation values. It is intended that experimental results will provide key data in the transition from simulation results to pilot scale with large scale industrial low carbon emission plant in mind.

Viscoelastic creep/stress relaxation to predict S_{hmin} magnitude in deep sedimentary rocks

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Abstract: Viscoelastic stress relaxation method is proposed to derive accurate magnitudes of least principal stress S_{hmin} at depth in deep sedimentary rocks. The technique depends either on short-duration laboratory creep (time-dependent deformation) response or indirectly on rock's microstructure (specific surface area S_{N2}) and mineral compositions. Primary creep is recorded under realistic subsurface conditions on rock samples with varying mineralogy, organic richness, and maturity. Because of the viscoelastic formalism, both the laboratory creep response, and the field-scale stress relaxation can be modelled with power-law functions of time involving the elastic compliance of the shale B , the time-dependence exponent n , and the amount of total strain ϵ . We reported for the first time a novel way to interlink between creep behaviour of rocks with their specific surface area as well as weak mineral phase *ClayTocPHI* composed of total clay, total organic content, and porosity. This fast and cost-effective indirect empirical method is utilised to check the predictive capability of S_{hmin} magnitudes across six lithological layers in an unknown prolific unconventional gas shale formation from predicted creep responses (B , n) along with the assumption of a relative in situ stress ratio ($\emptyset = \frac{S_2 - S_3}{S_1 - S_3}$), constant tectonic loading rate and geological age. Direct measurements of S_{hmin} magnitudes validate the proposed method and have able to capture the layered variation of stress with depth. On the other hand, conventional Eaton's extended model could not capture the stress layering effect precisely and may introduce more uncertainty because of its dependency on several unpredictable parameters.

Dual-phase with Ni addition: microstructure design and hydrogen embrittlement resistance evaluation

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Abstract: Dual-phase low alloy steels (DP LASs) are extensively used in the automotive industry due to their low cost and excellent mechanical and high technological properties. In addition, the ferrite and martensite microstructural features tailored by heat-treatment processing coupled with Ni additions make these steels promising candidates for hydrogen-related applications. Snape et al. studied DP LASs on a commercial-grade with Ni (AISI 4340 ~ 2%Ni), which showed superior mechanical properties and resistance to hydrogen environments when the microstructure was composed of ferrite and tempered martensite. Although its potential, Ni additions on LAS are restricted for hydrogen pipelines to 0.5% due to over-conservative standards based on experiences from the oil and gas industry, in which the failure mechanism's complexity exceeds the effect of hydrogen. As a result, hydrogen transport relies on over-dimensioned steels with relatively poor mechanical properties or expensive alloys, limiting economic and safe hydrogen delivery feasibility.

Research-grade DP LASs were designed to improve the hydrogen embrittlement (HE) resistance in this work. In addition, the role of Ni on the HE resistance was performed using in-environment slow strain rate test (SSRT) with varying Ni content and fixed ferrite-martensite ratio. Further, the hydrogen transport kinetics properties were evaluated by performing hydrogen permeation test, and the hydrogen trapping properties were studied using thermal desorption spectroscopy (TDS). Finally, microstructural characterization was performed by scanning electron microscopy (SEM). Ductility loss due to hydrogen embrittlement, hydrogen diffusion and trapping quantification were linked to improving the understanding of the role of Ni and microstructure on the HE.

EXPERIMENTAL HYDRAULIC FRACTURING TECHNIQUE FOR HARD ROCK IN-SITU RECOVERY ENHANCEMENT

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Abstract: The mining industry faces challenges, including declining ore grades, increases in operating depth, increases in cost, and environmental problems related to tailings and backfilling. In-situ recovery (ISR) offers an alternative approach to extract target minerals from deposits without costly processing. However, when an orebody is impermeable, the application of a stimulation technique, e.g., hydraulic fracturing, is necessary to artificially create conductive flow channels for the leaching agent, i.e., lixiviant, to contact the targeted mineral.

Rock mechanical properties, hydraulic fracturing parameters, and field conditions are the governing factors that determine the accessibility for ISR. Limited experimental information is available on hard rock leaching combined with hydraulic fracturing. In this work, a summary of conducted experimental trials that aimed at hard rock fracturing, including sample preparation, plus a sensitivity analysis of the governing fracturing factors are presented. Hydraulic fracturing fluid type, fluid injection rate, natural fracture distribution, and the variable stress strength and direction applied to hard rock samples were tested to evaluate their importance in ISR enhancement. The hydraulic fracture response with changes in fracturing pressure and its induced strain on the rock body will be included for evaluation. Outcomes from hydraulic fracturing experiments on hard rocks cover the hydraulic induced fracture geometry, strain data and X-ray computed tomography results. An extensive number of tests that combine test data monitoring and analysis will yield a better understanding in complex hard rock hydraulic fracturing processes, and the results provide practical guidance for further mining industrial practice.

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Long-and Short-term Strategies for Estimation of Hydraulic Fracturing Cost Using Fuzzy Logic

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Abstract: Block caving mining has recently applied hydraulic fracturing technique for a preconditioning method. Even though preconditioning method used in the practical case of usage, the cost estimation has difficulty for initial stage of budget sanction. Thus, this study aims to suggest the base case of specified costs of hydraulic fracturing based on the U.S. Energy Information Administration (EIA) report. Furthermore, hydraulic fracturing cost estimation applies cavability factor as the geological factor indicators to develop the long- and short-term strategies through the fuzzy inference system. In the long-term strategy, for reducing the long-term strategy's uncertainty, the cost estimation modelling considers the association for the advancement of cost engineering (ACE)'s contingency rate through three possible scenarios. Moreover, these scenarios are structured by each of fuzzy memberships and also redeveloped through arithmetic fuzzy operations over independent/dependent fuzzy numbers for identifying the uncertainty of dependence in the variables. The outcome of this study suggested decision process of the early stage of infrastructure and ore production by facilitating undercut propagation and controlling block height of block caving operation including additional fragmentation processes. The result of this study also illustrated that systematic fuzzy cost engineering with contingency rate could help estimate the initial stage of budgeting with reducing the uncertainty and identifying the systematic risk quantification.

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Poster presentations

Water Shutoff in High Permeability Sandstone Gas Reservoirs: Role of Additives and Fluid Flow Rate

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Abstract: Excessive water production has become a major challenge in gas reservoirs. Relative permeability modifiers (RPM) have been used to selectively reduce water production with minimum effect on the hydrocarbon phase.

1. In this manuscript we examined the effect of an additive (Aminopropyl–triethoxysilane) on the performance of the anionic polyacrylamide (PAM) as an RPM in a high permeability sandstone sample.

2. We also evaluated the performance of the treatments as a function of flow rate.

To achieve these objectives, core-flooding experiments have been conducted to measure water and gas permeabilities before and after successive treatment of PAM with and without the additive. A high permeability Bentheimer sandstone sample (2000mD) was used in our experiments. A 2%wt KCl solution and nitrogen were used as the liquid and gas phases, respectively. The applied range of water and gas flow rates (Q_w and Q_g , respectively) were 1-10 cm³/min. Water and gas residual resistance factors (F_{rw} and F_{rg} , respectively) were used to evaluate the performance of the treatments.

Treating the sample with 5000ppm then 15,000ppm PAM solutions resulted in F_{rw} around 2.5 and 1.4, respectively. Both treatments showed no water flow rate dependency. Under both treatments, F_{rg} remained approximately close to 1 as Q_g increases from 1 to 10 cm³/min. For possible improvement, we then treated the rock with 20,000ppm PAM solution premixed with 20,000ppm of earlier mentioned additive. A treatment with this solution resulted in F_{rw} around 5 (at 1-4 cm³/min Q_w). However, increasing Q_w to 10 cm³/min sharply reduced F_{rw} to 1.1. This treatment resulted in gas permeability improvement ($F_{rg}=0.57$) for some flow rates. A subsequent treatment with 40,000ppm PAM premixed with 40,000ppm of additive resulted in a large increase in both F_{rw} and F_{rg} with a significant dependence of F_{rw} on water flow rate (shear thinning). For instance, increasing Q_w from 1 to 10cm³/min decreased F_{rw} from 1000 to 37 while F_{rg} remained around 70. To conclude, Aminopropyl–triethoxysilane can improve the performance of RPM towards significant reduction in water permeability and gas permeability improvement. However, too much of the additives may have similar effect on F_{rg} . In addition, the PAM with additives seems to be more flow rate sensitive. Aminopropyl–triethoxysilane can significantly improve the performance of anionic polyacrylamide in reducing water permeability in high permeability reservoirs. In addition, this additive can even increase the permeability of gas phase after the treatment probably due to deforming the adsorbed polymer layer combined with reduction in the friction factor of the gas phase with pore surfaces.

An investigation of *in situ* formation of metal pyrophosphates (MP_2O_7 , where M = Sn, Ti and Zr) in PA/PBI based composite membrane in high-temperature polymer electrolyte membrane fuel cells

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Abstract: Fuel cells are electrochemical energy conversion devices to directly convert chemical energy of fuels such as hydrogen, methanol and natural gas to electricity with very low greenhouse gas emission and high efficiency. Among them, the state-of-the-art phosphoric acid (PA) doped polybenzimidazole (PBI) based proton exchange membrane fuel cell (PEMFCs) has shown excellent long-term stability up to 18000 h at 160 °C. Beside of this, increasing the operating temperature to 200-300 °C has attract significant interest to take advantages of simplified water management system, high CO tolerance and the possible integration with methanol reformers. However, PA/PBI based PEMFCs still process the limitation of inevitable PA leakage from membrane at elevated temperature, which also results in the issue of Pt catalyst poisoning in electrodes. Herein, we report the development of *in situ* formed metal pyrophosphates (MP_2O_7 , where M = Sn, Ti and Zr) in PA/PBI composite membranes for HT-PEMFCs. The *in situ* formed MP_2O_7 /PA/PBI composite membranes show significantly improved performance and stability under the operation conditions at 200 mA cm^{-2} and 250 °C for over 50 h. In addition, compared with *in situ* formed TiP_2O_7 /PBI/PA and ZrP_2O_7 /PBI/PA composite membranes, its best durability performed under accelerated stress test (AST) is associated with the highest acid retention ability and the uniform distribution of *in situ* formed SnP_2O_7 nanoparticles in PBI matrix, which shows a promising capability to alleviate the PA leaching at elevated temperature.

Maleic anhydride based polymeric additives for the control of flow assurance problem of gas hydrate formation

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Abstract: Gas hydrate formation in oil and gas transportation facilities is one of the major flow assurance problems and needs attention as this problem incur capital investment and operational downtime. Due to large quantity application of thermodynamic gas hydrate inhibitors, concentration is increasing on application of low-dosage inhibitors. Kinetic hydrate inhibitors (KHIs) are a kind a of low dosage inhibitor, which not only prevents or delays the gas hydrate nucleation, but also delays the hydrate crystal growth. In this research work, maleic anhydride based polymeric additives have been evaluated as KHIs. Maleic anhydride is widely and easily available low-cost material and it was allowed to react with organic acids (linoleic acid and ricinoleic acid) extracted from plant-based oils to develop two polymeric additives, which were already evaluated as pour point depressants in our previous research work. The two developed polymeric additives are poly (n-dodecyl linoleate –co- succinic anhydride) and poly (n-dodecyl ricinoleate –co- succinic anhydride), which will be denoted as MALN and MARC respectively. After, evaluation of MALN and MARC as KHIs in the current work, the two polymers would be termed as dual function inhibitor for wax as well as hydrate formation prevention. MALN and MARC were tested on a crude oil in water emulsion system including tetrahydrofuran (THF) for analysis of their hydrate prevention capacities. The tests on the THF model hydrate system were performed using a self-fabricated setup for hydrate induction time studies based on visual and temperature augmented method, with additive concentrations of 0.1, 0.3, 0.5, 0.7 and 1.0wt% of both MALN and MARC separately on experimental solutions containing water ratio of 70%, 80% and 90% in the emulsions. The test results reveal that both MALN and MARC acted as KHIs by delaying the hydrate induction time up to 18 hours at 1.0wt% concentrations, which was only 8 minutes without any inhibitor. Also, the hydrate agglomeration times were recorded as beyond 24 hours at 1.0wt% concentrations, indicating excellent performance of the two laboratory synthesized additives. Thus, two synthesized polymeric additives may be considered as a potential low dosage hydrate inhibitor of KHI category for prevention of hydrate formation during crude oil pipeline transportation.

CFD Analysis of Frost Growth under Various Conditions using Mass Transfer Theory

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Abstract: Frost formation is a phenomenon that occurs when the temperature of water vapor drops below its dew point and equilibrium freezing temperature. In industrial heat exchanger applications, the presence of frost reduces the heat transfer efficiency by adding a layer of thermal resistance and increases the pressure drop by restricting flow passages. Hence, understanding and predicting frost layer growth and its properties have been a topic of study for decades. Numerous experiments have been conducted to observe frost formation, followed by mathematical models to predict its growth in thickness and density, as well as its properties. However, most of the existing predictive models use empirically fitted coefficients to force agreement between the mathematical model and experimental data. Consequently, the usability of those models is restricted to the conditions at which they were tuned to.

In this study, a multiphase Computational Fluid Dynamics (CFD) model to predict frost formation under refrigeration conditions (temperatures below -20°C) was developed. The need for empirically fitted coefficients in the mass transfer rate equations was eliminated, and dimensionless numbers derived from mass transfer theory were used to develop a more generic model. The mass transfer equation is driven by the supersaturation degree of water vapor in the air. The model was validated against experimental data under a range of different conditions, i.e., varying cold surface temperatures, air humidities and air temperatures.

The model achieved $\pm 20\%$ accuracy when compared to experimental data. The thickness of the frost growth follows the 0°C thermal iso-surface, which in turn is affected by the operating conditions and the heat transfer from the cold surface through the frost layer. Qualitatively, the behavior of frost layer growth under different conditions were also successfully shown by the model. As the surface temperature becomes colder, the frost layer formed is thicker but less dense. This can be explained by the mass transfer contours shown in the simulation that at colder surface temperatures, frost formation rate is higher at two localized regions, which are directly on top of the cold surface and at the air-frost interface, resulting in a quicker frost thickness growth but a slow densification process. Apart from that, the model predicted that frost thickness increases with increasing air humidities and decreasing air temperatures.

The generic multiphase model has shown that it is capable of predicting frost formation at refrigeration temperature under different conditions, making it suitable for predicting frost formation in real-world applications. The next step of this study will be to expand the model's capability to predicting frost formation under cryogenic conditions (temperatures below -150°C).

Effect of Wire Shape and Size in Droplet Capture

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Abstract: The droplet impact and capture on a thin wire is the key governing phenomena in a great number of separation processes, especially in mist elimination processes that require the use of knitted mesh pads. The performance of the knitted mesh is governed by the hydrodynamics of droplet impact. Understanding the fundamentals of the hydrodynamic phenomena and numerical representation of droplet impact on a thin wire is of great importance to predict the parameters that govern the capture of droplets. For a given wire and droplet size, there is a maximum impact velocity that results in droplet capture or a hanging droplet on a horizontal, stationary wire ($V_{t,max}$). This study investigates the effect of various shapes and sizes of wires on the $V_{t,max}$. Computational Fluid Dynamics (CFD) models were developed with a computational domain of 3 mm in width and 6 mm in height. A 200 μm droplet was patched at 0.5 mm below the wire and exposed to a continuous upward airflow at different velocities (0.25 m/s – 4 m/s). Four shapes of wires were investigated; this includes a circle, a square, an equilateral triangle, and an inverted equilateral triangle along with three different wire sizes (0.25 mm, 0.5 mm, and 1 mm). The mass of water attached to the surface of the wires was measured at a steady-state (as shown in Fig 1). The droplet impact phenomena were analysed by quantifying the mass of the water attached to the wire surface and evaluating the maximum terminal velocity of each shape.

Natural Hydrogen Prominence and Controls of Distribution in the Earth Crust

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Abstract: The studies of natural, or subsurface, sources of hydrogen are gaining momentum among the scientific and industrial community. With immense flow of field and experimental data from all directions, it is becoming apparent that there is an urgent need for fresh, alternative insight into the very core of fundamental geology science, with the purpose of taking this new data into account and attempting to resolve numerous dilemmas and paradoxes, at times quite disturbing, accumulated by this discipline through the past several decades.

This work is an attempt to identify and classify the principles of natural hydrogen provenance and distribution within the lithosphere as well as its manifestations on the surface. While explaining the scientific basics of the subject in commonly acceptable terms, the author will try to concentrate on the practical implications and outcomes.

This study's purpose is to analyze the known natural hydrogen cases in Australia and around the globe. The main controls, such as structural, stratigraphical, lithological, geochemical, and tectonic elements will be reviewed and ranked. The commonly accepted points will be confirmed or, otherwise, questioned and debated.

Since the modern resource exploration industry is capable of employing quite sophisticated and versatile techniques and instruments, it is very important to assess and confirm their suitability for the natural hydrogen application. Similar to the oil and gas industry some 150 years ago, it is time to switch from assessing the surficial manifestations of natural hydrogen to sub-surface methods and tools, in order to provide the industry with reliable exploration technology.

Comparison study of methanol production via CO₂ hydrogenation and syngas

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Abstract: Methanol synthesis is highly exothermic and equilibrium-controlled reaction. The process is primarily governed by the heat transfer and conversion of the reactor. There are two types of reactor for methanol synthesis, adiabatic and isothermal reactor. Adiabatic reactor typically comprises of multi-stage reactor with intermediate cooling and has low per-pas conversion. While isothermal reaction, provide higher yield performance but it has more complexity. In this paper, an isothermal reactor was chosen as based of optimisation for two different methanol synthesis pathway, CO₂ hydrogenation and syngas. The performance was compared with each tubular reactor scenario. Figure 1a and b shows the comparison of the performance for isothermal reactor for CO₂ hydrogenation and syngas, respectively. When the syngas pathway was used the temperature was significantly higher compare to the CO₂ hydrogenation. The syngas pathway could reach about 590K peak at the beginning of the reaction while CO₂ hydrogenation only reached 530K. The axial profile also reaching stagnant profile around 525K. Similarly, the syngas pathway also having stagnant temperature profile at 525K after reaching its peak at 590K. In terms of yield profile, the syngas pathway produced significantly higher methanol flow compare to the CO₂ hydrogenation. The syngas produced about 0.016 mol/s of methanol while CO₂ hydrogenation only produced around 0.0075 mol/s of methanol. The Syngas which comprise of mixture of CO₂, CO and H₂ offers more conversion pathway of carbon compare to CO₂ hydrogenation which solely depends on the conversion of CO₂. This was shown by the temperature profile of syngas reaction to methanol which has higher peak. The Hydrogenation of CO to methanol is significantly exothermic at -128 kJ/mol. While the CO₂ hydrogenation also produce CO as the intermediate (in RWGS), CO was not converted into methanol which resulting in lower total yield produced. With the same reactor and space velocity, the production of methanol via syngas is benefiting more in terms of yield. While CO₂ hydrogenation offer more steady temperature profile but in expenses of lower methanol yield which is not favourable in industrial setting.

Adsorption of CO₂/CH₄ Mixtures in Activated Carbon

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Abstract: Carbon dioxide (CO₂) adsorption by activated carbon (AC) is a widely applied approach in industrial natural gas separation and purification. The design and optimization of the processes depend on the understanding of mechanisms of multicomponent adsorption, especially for CO₂/CH₄ mixtures. With the development of computational technology, molecular simulation becomes a useful tool and can be an important compensation for experimental measurement when investigating the mechanisms microscopically. In the simulation, AC is commonly modelled as graphitic slit pores with a uniform pore size distribution, which are far simplified considering the complex pore configuration in real AC. Therefore, recently, the wedge pore has been proposed as a more realistic model for representing the non-uniformity of AC as its size is continuously changing in the axial direction. To evaluate this wedge pore model, in this work, the isotherms of binary CO₂/CH₄ mixtures adsorption in AC at 298 K obtained with wedge pore models will be collected and compared against the simulation results of the slit pore model, the experimental data and the prediction obtained with the Ideal Adsorption Solution Theory (IAST). The wedge pore model to some extent gives a better prediction compared to the slit pore model and has comparable results with the IAST, especially in the low-pressure region. The multicomponent adsorption predictions of the wedge pore model were also well fitted or were close to the experimental data than the slit pore model, which justifies using the wedge pore model as a more realistic model for representing the AC.

Selected Photos



Group Photo



Best Oral presentation award- Marcos Exequiel Arguello



Best poster Presentation award- Joshua C. Q. Wong



Opening session- A/Prof Hussein Znad



Opening session- Prof Michael Hitch



Opening session- Prof Kate Trinajstic



Industry Keynote speaker- Amanda Panting (Woodside)



Industry Keynote speaker- Mr. Tony Tang- (Blackstone Minerals)



Industry Keynote speaker- Dr. Sofia Hazarabedian (KBR)



Industry Keynote speaker- Mr. Ivor Bryan (Mining & Process Solution)



Industry Keynote speaker- Mr. Andrew Tran (Schlumberger Australia)



